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Temperature variation of Debye-Waller factor and mean square displacement for some transition metals

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Abstract : Debye-Waller factors and mean square displacements at different temperatures for ten fcc transition metals (Cu, Ni, Fe, Co, Ag, Pd, Rh, Au, Pt and Ir) have been computed on the basis of a lattice mechanical model proposed recently by Antonov *et al* [*Z Phys B-Condensed Matter* 79 223, 233 (1990)]. The theoretical values are compared with those recently obtained from experimental density of states by Peng *et al* [*Acta Cryst* A52, 456 (1996)]. A satisfactory agreement between theory and experiment has been found For Ir and Rh the theoretical values have predictive meaning.

Keywords Transition metals, Debye-Waller factor, mean square displacement

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Recently, Antonov *et. al.* [1, 2] have proposed a pseudopotential model approach for the lattice mechanical properties of fcc transition metals. In this approach, the contribution of *s*-like electrons is calculated in the second order perturbation theory for the local model pseudopotential while that of the *d*-like electrons is taken into account by introduction of repulsive short range interatomic potential. The model was applied to ten transition metals (Cu, Ni, Fe, Co, Ag, Pd, Rh, Au, Pt and Ir). This model was used for the calculations of phonon dispersion curves, density of phonon states, elastic constants and their pressure derivatives, Interatomic interaction, variation of Debye temperature with temperature, mode Gruneisen parameters, temperature variation of Gruneisen parameter and cold equation of state with reasonable success. Encouraged by this fact, we undertake the computations of temperature variation of Debye-Waller factors and mean square displacements for these metals. In this report, we present the results of our calculations and compare them with the recent data given by Peng *et. al.* [3].

In the harmonic approximation, the Debye-Waller exponent 2W is directly obtained from the computed phonon density of states [4]. If $g(\nu)$ is the frequency distribution function for the phonons giving the number of vibrational modes in the frequency interval between ν and $\nu + d\nu$, then

$$2W_T = \frac{8\pi^2\hbar}{3MN}\left(\frac{\sin\theta}{\lambda}\right)^2 \int_0^{\nu_{max}} \frac{g(\nu)}{\nu} \coth\left\{\frac{h\nu}{2k_BT}\right\} d\nu, \quad (1)$$

where θ is the glancing angle and λ is the wave length of incident radiation. M is mass of the atom and N denotes the total number of unit cells in the crystal. In the harmonic approximation, the mean square displacement of the atoms in the crystal is given by the relation

$$\overline{U}^2 = \frac{3}{8\pi^2}\left(\frac{}{\sin\theta}\right) W_T \quad (2)$$

The frequency spectra of the lattice vibrations of all the ten metals considered here were computed by the numerical sampling of frequencies according to Blackmann's technique [5-7]. In the present work, we have considered a mesh of evenly spaced 64000 wave vectors in the first Brillouin zone. The details of the calculations may be found in ref [4]. The expressions for Dynamical matix and numerical values of model parameters were taken from Ref [4].

We present in Figures 1 and 2, the Debye-Waller factors and mean square displacements for Cu, Ag, Co, Rh and Ir. We also

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display in the same figures, the same quantities as obtained recently from the experimental phonon density of states by Peng *et al* [3]. The results for other metals (Au, Ni, Pd, Pt and Fe) are

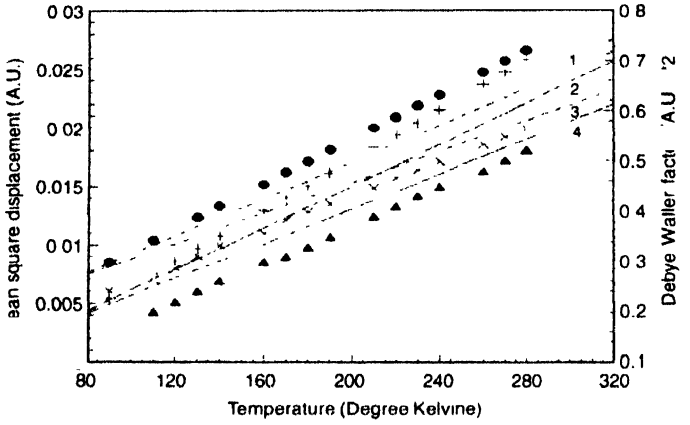

Figure 1. Temperature variation of Debye-Waller factor W_T and mean square displacement $\langle u^2 \rangle$ for atoms of Cu and Ag Continuous lines 2 and 4 represent theoretical results of W_T for Ag and Cu respectively Experimental results (+) and (▲) are from Peng *et al* [3]. Dotted lines 1 and 3 represent theoretical results of $\langle u^2 \rangle$ for atoms of Ag and Cu Experimental results (●) and (x) are from Peng *et al* [3]

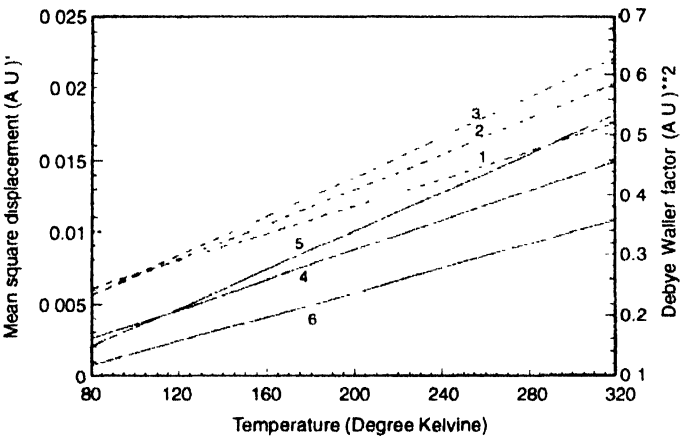

Figure 2. Temperature variation of Debye-Waller factor W_T and mean square displacement $\langle u^2 \rangle$ for atoms of Co, Ir and Rh. Continuous lines 4,5,6 represent theoretical results of W_T for Co, Ir and Rh respectively Dotted lines 1,2,3 represent theoretical results of $\langle u^2 \rangle$ for Co, Ir, Rh respectively.

similar and hence we do not give these results in the form of graphs. The maximum deviations from experimental results for these metals are given in table [1]. The overall agreement in each case is quite satisfactory. Particularly, the presently studied model due to Antonov *et. al.* [1, 2] works quite well for Ag, Au, Pd & Pt metals. For Cu, Ni and Fe, the maximum deviation of about 25 – 30% occurs only at a very small number of points. For most of the temperatures, the theoretical results agree with experiments to within about 12 – 15%. The anharmonic effects, in the case of Ni and Fe, are seen to be important beyond about 200 K. As stated in the introduction, the pseudopotential approach as proposed by Antonov *et al* [1, 2] has been successful in reproducing reasonably well the phonon frequencies [8, 9] and cold equation of states of Ir and Rh right up to 40% compression ; we believe that our computed values of Debye-Waller factors and mean square displacement for Ir and Rh being reported for the first time, may be considered as fairly good estimates.

Table 1. The maximum deviation of calculated values of W_T and $\langle u^2 \rangle$ from experimental results for Cu, Ag, Au, Ni, Pd, Pt and Fe

Metal	Maximum % deviation for W_T	Maximum % deviation for $\langle u^2 \rangle$
Cu	30	30
Ag	12	11
Au	6	6
Ni	26	28
Pd	12	14
Pt	13	13
Fe	16	25

We have presented in this report, the results of calculations of Debye-Waller factors and mean square displacements of ten fcc transition metals. The model approach, we used, is that due to Antonov *et al* [1, 2]. This model approach has been successful in predicting many lattice mechanical properties of these metals We have extended the range of applicability of this approach by computing the Debye-Waller factors and mean square displacement.

Despite the importance of the Debye-Waller factor in dynamical electron diffraction calculations, accurate values of the Debye-Waller factors are not readily available for most crystals. Experimentally, the Debye-Waller factors may be measured using such techniques as neutron or X-ray diffraction However, the experimental results are normally published at one temperature [10], which does not correspond exactly to the experimental situation under which an electron microscopy experiment is normally conducted. It is in this circumstance, a reasonable model approach to calculate this quantity is highly desirable. In the present report, we have successfully explored the possibility of using for this purpose, the model approach due to Antonov *et al* [1,2].

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